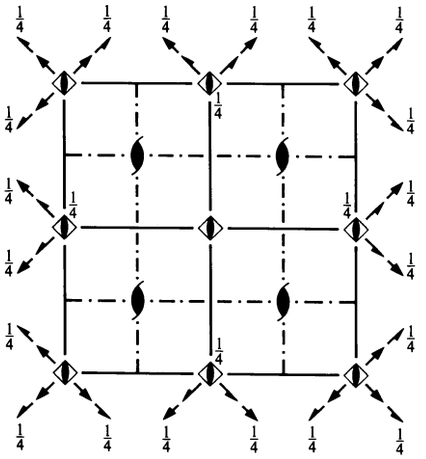
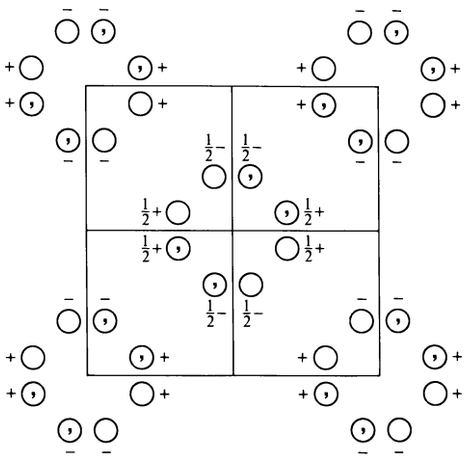
Tetragonal $\bar{4}m2$ D_{2d}^{9} $I\bar{4}m2$

Patterson symmetry $I4/mmm$ $I\bar{4}m2$ No. 119





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) m $x,0,z$	(6) m $0,y,z$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
8	i	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$
8	h	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$
8	g	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$
4	f	$2\,m\,m.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$		
4	e	$2\,m\,m.$	$0,0,z$	$0,0,\bar{z}$		
2	d	$\bar{4}\,m\,2$	$0,\frac{1}{2},\frac{3}{4}$			
2	c	$\bar{4}\,m\,2$	$0,\frac{1}{2},\frac{1}{4}$			
2	b	$\bar{4}\,m\,2$	$0,0,\frac{1}{2}$			
2	a	$\bar{4}\,m\,2$	$0,0,0$			

Reflection conditions

General:

hkl: $h+k+l=2n$
$hk0$: $h+k=2n$
$0kl$: $k+l=2n$
hhl: $l=2n$
$00l$: $l=2n$
$h00$: $h=2n$

Special: no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

